REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

1. REPORT DATE *(DD-MM-YYYY)*	2. REPORT TYPE	3. DATES COVERED *(From - To)*
10-26-1999	Final Technical Report	1998 Aug 01 - 1999 Jul 31

4. TITLE AND SUBTITLE
"Final Report for STTR AF98T010 - Upgrading the Field-Particle Physics and Numerics of PIC codes for HPM Tube Design"

5a. CONTRACT NUMBER
F49620-98-C-0044

5b. GRANT NUMBER
STTR AF98T010

5c. PROGRAM ELEMENT NUMBER

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5d. PROJECT NUMBER
FQ8671-9801369 STTR/TS

5e. TASK NUMBER

5f. WORK UNIT NUMBER

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
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8. PERFORMING ORGANIZATION REPORT NUMBER
1

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)
USAF, AFMC
Air Force Office of Scientific Research
110 Duncan Avenue, Room B115
Bolling AFB, DC 20332-8050

10. SPONSOR/MONITOR'S ACRONYM(S)
AFOSR

11. SPONSOR/MONITOR'S REPORT NUMBER(S)
0002AA

12. DISTRIBUTION/AVAILABILITY STATEMENT
Distribution Statement A. Approved for public release; distribution is unlimited.

13. SUPPLEMENTARY NOTES
Not applicable

14. ABSTRACT
The primary objective of this contract was to deveop an understanding from first principles of the macroscopic particle force equation arising from the microscopic particle and field interaction dynamics and to incorportate those effects in a self-consistent state-space (rate equation) particle-in-cell (PIC) calculation. Effective current and charge density time-domain equation models were to be developed from this generalized Lorentz force model. Also to be developed in this project were the numerical modeling techniques that would allow the self-consistent coupling of the particle motions and the evolution of the electromagnetic fields in the presence of complex electrmagnetic scatterers. The resulting simulators were to be applied to a variety of high power microwave (HPM) source configurations. The specific tasks considered during the contract period included: 1. develop a generalized Lorentz force equation to include sef-forces on the particles and to develop its equivalent current and charge rate equeations directly in the space-time domain; 2. develp the PIC tools and techniques for modeling the interaction of intense electromagnetic fields with one or several particles in one, two, and three space dimensions and time; 3. apply the resulting simulators to study the generation of microwaves in a HPM source cavity, particularly by predicting any additional microscopically-derived force effects on a large.....

15. SUBJECT TERMS
Particle-in-cell (PIC), Hign power microwave (HPM) tube design, field-particle physics

16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	18. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
a. REPORT	b. ABSTRACT	c. THIS PAGE			Dr. Arthur Yaghjian
U	U	U	UU	22	19b. TELEPHONE NUMBER *(Include area code)* 617-424-9295

October 1999 Final Report for STTR AF98T010

Upgrading the Field-Particle Physics and Numerics of PIC codes for HPM Tube Design

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ABSTRACT

The primary objective of this contract was to develop an understanding from first principles of the macroscopic particle force equation arising from the microscopic particle and field interaction dynamics and to incorporate those effects in a self-consistent state-space (rate equation) particle-in-cell (PIC) calculation. Effective current and charge density time-domain equation models were to be developed from this generalized Lorentz force model. Also to be developed in this project were the numerical modeling techniques that would allow the self-consistent coupling of the particle motions and the evolution of the electromagnetic fields in the presence of complex electromagnetic scatterers. The resulting simulators were to be applied to a variety of high power microwave (HPM) source configurations.

The specific tasks considered during the contract period included:

1. develop a generalized Lorentz force equation to include self-forces on the particles and to develop its equivalent current and charge rate equations directly in the space-time domain;

2. develop the PIC tools and techniques for modeling the interaction of intense electromagnetic fields with one or several particles in one, two, and three space dimensions and time;

3. apply the resulting simulators to study the generation of microwaves in a HPM source cavity, particularly by predicting any additional microscopically-derived force effects on a large number of charged particles; and

4. apply the resulting simulators to study a many-particle plasma system typically found in HPM sources.

1 INTRODUCTION

The starting point of all physical-space and physical-time PIC codes is to divide space and time into discrete cells, i.e., form a space-time grid or lattice. The continuum differential equations describing the evolution of the fields and particles are given, for instance, in the non-relativistic limit by the Maxwell-particle system

$$\begin{aligned}
\partial_t \vec{H} &= -\frac{1}{\mu} \nabla \times \vec{E} \\
\partial_t \vec{E} &= \frac{1}{\epsilon} \nabla \times \vec{H} - \frac{1}{\epsilon} \vec{J} \\
\partial_t \vec{r} &= \vec{v} \\
\partial_t \vec{v} &= \frac{q}{m} \left(\vec{E} + \mu \, \vec{v} \times \vec{H} \right) \\
\\
\nabla \cdot (\epsilon \vec{E}) &= \rho \\
\nabla \cdot (\mu \vec{H}) &= 0 \\
\vec{J} &= \rho \vec{v}
\end{aligned} \tag{1}$$

where the charge density is determined by the individual particle locations through the expression

$$\rho(\vec{r}) = \sum_j q_j \delta^{(3)} \left(\vec{r} - \vec{r}_j \right) . \tag{2}$$

In a PIC code the charged particles q_j are tracked individually (by calculating their trajectories $\vec{r}_j$) and their contributions to the total electromagnetic field are self-consistently calculated with that field.

To numerically implement this system of equations, one must assign all of the field and charge quantities to the discrete grid. The typical approach is to use a 0 grid finite difference approximation for all of the 0. This leads to a second order accurate system of equations of the form:

$$
\begin{aligned}
\vec{H}^{(n+1/2)} &= \vec{H}^{(n-1/2)} - \frac{\Delta t}{\mu}\left(\nabla \times \vec{E}^{(n)}\right) \\
\vec{v}^{(n+1/2)} &= \vec{v}^{(n-1/2)} + q\,\vec{E}^{(n)}\,\Delta t \\
&\quad + \frac{q}{4m\mu_0}\left(\vec{v}^{(n+1/2)} + \vec{v}^{(n-1/2)}\right) \times \left(\vec{H}^{(n+1/2)} + \vec{H}^{(n-1/2)}\right)\Delta t \\
\vec{r}^{(n+1)} &= \vec{r}^{(n)} + \vec{v}^{(n+1/2)}\,\Delta t \\
\rho^{(n+1)}(\vec{r}) &= \sum_j q_j \delta^{(3)}\left(\vec{r} - \vec{r}_j^{(n+1)}\right) \\
\vec{J}^{(n+1/2)} &= \frac{1}{2}\left(\rho^{(n+1)} + \rho^{(n)}\right)\vec{v}^{(n+1/2)} \\
\vec{E}^{(n+1)} &= \vec{E}^{(n)} + \frac{\Delta t}{\epsilon}\left(\nabla \times \vec{H}^{(n+1/2)}\right) - \frac{\Delta t}{\epsilon}\vec{J}^{(n+1/2)}\,.
\end{aligned}
\tag{3}
$$

Much of the art associated with this discrete approach rests in the allocation of the particles to a cell in the grid, hence, the name PIC codes. There are many variations on this scheme. This differential equation set describes the motion of a charged particle in the presence of an electromagnetic field. Typically each numerical particle actually represents a composite number of real particles and these macro-particles are distributed in the cells of the grid at the positions $\vec{r}$. These macro-particles are then pushed in the grid by the electromagnetic field $\vec{E}, \vec{H}$; the charges in motion then modify the electromagnetic field. The process of field-solve and particle-push are usually taken in a two-step process. The moving charges are used to define the charge density ρ and the current $\vec{J}$ everywhere in space-time. The fields are

then obtained from these charges and currents. The resulting fields are in turn used in the force equation to push the charges. This leads to new charge densities and currents. The process is repeated through all the time steps in the simulation [1], [2], [3]. The algorithm thus proceeds in the following fashion:

- calculate $\vec{H}$ updates
- calculate the velocity updates from the Lorentz force
- calculate the updates for the location of the particles
- calculate the new charge and current densities
- calculate $\vec{E}$ updates
- repeat this cycle.

Because space is discretized and the electromagnetic properties of the medium in which the particles are moving are assigned to each cell in the grid, very complex structures and materials can be handled with a PIC code. The major costs in a PIC code comes from the particle-push stage ($\sim$ 90% of the simulation time). The field-solve is quite efficient ($\sim$ 10% of the simulation time). Unfortunately, the larger the number of particles, the better the overall simulation results will be. This leads to very time consuming and costly calculations. Nonetheless, these PIC codes have been very effective in the design of many high power microwave (HPM) tubes and in the modeling of HPM effects associated with the large fields generated with these tubes. However, with the need to decrease the sizes of the sources while increasing their outputs, more exact numerical models of the microwave generation process are desired.

One very interesting point is that many codes assign the particles to the grid cells through an interpolation or weighting scheme. As Birdsall [2] indicates, the grid charge density ρ_j can be obtained from the charges q_j located at the positions $\vec{r}_j$ from the expression

$$\rho(\vec{r}_j) = \sum_i q_i \mathcal{S}\left(\vec{r}_j - \vec{r}_i\right) \tag{4}$$

where $\mathcal{S}$ is a shape function which weights (interpolates) the particles which are found within a cell to their appropriate edge or node locations in the 0 grid finite difference scheme. The particles themselves are assumed to have finite size (macro-particles). Similarly the electric force on the particle q_j takes the form

$$\vec{F}_j(\vec{r}_j) \;=\; q_j \sum_i \mathcal{S}\left(\vec{r}_j - \vec{r}_i\right) \vec{E} \cdot d\vec{l}_i \tag{5}$$

where $d\vec{l}_i$ is the oriented length of the cell edge at $\vec{r}_i$. Because the weighting functions on the force and the charge density are typically selected to be the same, symmetric difference equations relating $\rho(\vec{r})$ and $\vec{E}(\vec{r})$ in space result and ensure the conservation of momentum. This approach, in fact, eliminates the effects of the self-forces.

If the fields are of sufficient strength, the plasma must be treated in a relativistic sense. One finds that if the relativistic momentum of a particle of rest mass m_j and charge q_j is

$$\vec{p}_j \;=\; \gamma_j m_j \vec{v}_j \tag{6}$$

where the relativistic term is given by

$$\gamma_j \;=\; \left(1 - \frac{v_j^2}{c^2}\right)^{-1/2} = \left(1 + \frac{p_j^2}{m_j^2 c^2}\right)^{1/2} \tag{7}$$

then the equations of motion of its position $\vec{r}_j$ and momentum $\vec{p}_j$ are

$$\begin{aligned}
\frac{d}{dt}\vec{r}_j &= \vec{v}_j = \frac{\vec{p}_j\, c}{(m_j^2 c^2 + p_j^2)^{1/2}} \\
\frac{d}{dt}\vec{p}_j &= q_j \left[\vec{E} + \vec{v}_j \times \vec{B}\right] = q_j \left[\vec{E} + \frac{\vec{p}_j}{\gamma_j m_j} \times \vec{B}\right] \\
\vec{v}_j &= \frac{\vec{p}_j}{\gamma_j\, m_j} = \frac{\vec{p}_j\, c}{(m_j^2 c^2 + p_j^2)^{1/2}} \,. \qquad (8)
\end{aligned}$$

The update equations become more complex because the Lorentz force equation becomes explicitly nonlinear with the presence of the relativistic term γ_j. Since it depends on the momentum, the relativistic term γ_j must be varied at each time step too [3]. A variety of schemes exist to handle these relativistic considerations. One straight-forward approach requires solving for an update in γ_j at each time step through the conservation of energy, i.e.,

$$\frac{d}{dt}\psi_j = \frac{d}{dt}\left(\frac{1}{2}\gamma_j^2\right) = \frac{q_j}{m_j^2 c^2}\, \vec{p}_j \cdot \vec{E} \,. \qquad (9)$$

Other approaches include approximations which involve using the values of the velocity at the previous time step or some average between the current and previous values.

Whichever scheme is used, the basic update equation set then takes the form

$$\begin{aligned}
\vec{H}^{(n+1/2)} &= \vec{H}^{(n-1/2)} - \frac{\Delta t}{\mu}\left(\nabla \times \vec{E}^{(n)}\right) \\
\psi_j^{(n+1/2)} &= \psi_j^{(n-1/2)} + \frac{q_j}{m_j^2 c^2}\, \vec{p}_j^{(n)} \cdot \vec{E}^{(n)}
\end{aligned}$$

$$
\begin{aligned}
\vec{p}_j^{(n+1)} &= \vec{p}_j^{(n)} + q_j \vec{E}^{(n)} \Delta t \\
&\quad + \frac{q_j}{4\mu_0 \gamma_j^{(n+1/2)} m_j} \left(\vec{p}_j^{(n+1)} + \vec{p}_j^{(n)} \right) \times \left(\vec{H}^{(n+1/2)} + \vec{H}^{(n-1/2)} \right) \Delta t \\
\vec{r}_j^{(n+1)} &= \vec{r}_j^{(n)} + \frac{1}{2} \left(\vec{p}_j^{(n+1)} + \vec{p}_j^{(n)} \right) \Delta t \\
\rho^{(n+1)}(\vec{r}) &= \sum_j q_j \delta^{(3)} \left(\vec{r} - \vec{r}_j^{(n+1)} \right) \\
\vec{J}^{(n+1/2)} &= \frac{1}{4\gamma_j^{(n+1/2)} m_j} \left(\rho^{(n+1)} + \rho^{(n)} \right) \times \left(\vec{p}_j^{(n+1)} + \vec{p}_j^{(n)} \right) \\
\vec{E}^{(n+1)} &= \vec{E}^{(n)} + \frac{\Delta t}{\epsilon} \left(\nabla \times \vec{H}^{(n+1/2)} \right) - \frac{\Delta t}{\epsilon} \vec{J}^{(n+1/2)}
\end{aligned}
\tag{10}
$$

where, of course, $\gamma_j^{(n+1/2)} = \sqrt{2\psi_j^{(n+1/2)}}$. The particle-push and field-solve algorithm proceeds as in the non-relativistic case.

The development of a full-wave, vector Maxwell and generalized particle force equation simulator is key to the success of modeling the interaction of the intense electromagnetic fields with the plasmas found in HPM sources. The strengths of finite difference methods lie in their geometry modeling flexibility due to their subdomain (grid cell) structure and the ability for one to couple efficiently the numerical models of diverse space and time scales.

However, one of the drawbacks of most PIC codes is the lack of the detailed microscopic dynamics in the particle motion. It does a simple Lorentz force action only. It does not include any additional particle effects such as the radiation reaction force and the collisions between the particles. Since a PIC simulation results in a description of the collective or average motion of many particles in the electromagnetic fields, a PIC simulation generally assumes that the averages of the particle motions will average-out these additional effects. At

high velocities, hence, high kinetic energies and over very small distances that are comparable to the microwave wavelength being generated, this assumption is not strictly correct.

One way in which more complex forces have been included in previous PIC calculations has been to include additional forces in the particle-push equations. A variety of methods have been introduced to model the electron-electron and electron-ion collisions including transforming to the spectral domain to deal with modifications of the Fourier components and introducing Monte Carlo calculations during the particle-push phase. Many of these techniques have difficulties because they restrict the applicability of the simulation space (periodic boundary conditions to handle the fast Fourier transforms) and introduce particle noise (additional randomness in the particle velocities).

One of the first efforts of the project was to assess the magnitude of the effects of the self-force on a PIC calculation. Additionally, alternative schemes for writing the continuum equations were considered with the hope that one would lead to a more self-consistent numerical scheme. A PIC code was obtained to run test problems that could reveal any discrepancies with basic plasma theories. The results of these efforts are summarized in the next section.

2 RESULTS

The primary objective of this phase-one project was to develop a refined understanding of the physical processes required in a PIC calculation to accurately model microwave generation in a HPM source. A variety of physical processes were considered including self-forces and forces between the background plasma and the more energetic electrons.

In Subsection 2.1 of this section we show that the self-force on electrons in linear high-

power microwave (HPM) devices is negligibly small compared with the relativistic Newtonian acceleration force. In Subsection 2.2 we show that this result also implies that the self-force on groups of electrons in the cells used for particle-in-cell (PIC) computer code calculations is also negligible. In 1 2.3 we prove that the self-force on a charge moving in the direction of a constant, uniform electric field is zero, and thus its motion is completely determined by the relativistic version of Newton's second law of motion. Lastly, in Subsection 2.4 this equation of motion is solved for the final velocity of an electron traveling in the uniform electric field between two oppositely charged parallel plates.

2.1 Estimate of the Effect of the Self-Force on Electrons in High-Power Microwave Devices

To correctly determine the electrodynamics of charged particles, one must, in general, take into account both the fields radiated by the accelerating charges and the self-force experienced by each of the charges [4]. Consider a high-power microwave device containing electrons traveling in approximately straight lines with an average speed u_0 that can be close to the speed of light c, as shown in Figure 1. Assume that the HPM device is operating at a frequency ω. In the laboratory inertial frame of reference, the Lorentz-Abraham-Dirac equation of motion of each electron can be written as [4, eq. (5.12a) and sec. 8.7]

$$F_{ext} = m\frac{d}{dt}(\gamma u) - \frac{e^2}{6\pi\epsilon c^3}\gamma^4\left[\frac{d^2u}{dt^2} + \frac{3\gamma^2}{c^2}u\left(\frac{du}{dt}\right)^2\right] \tag{11}$$

where $u(t)$ is the instantaneous velocity of the electron

$$\gamma = \frac{1}{\sqrt{1-u^2/c^2}} \tag{12}$$

and m and e are the rest mass and charge of the electron, respectively. The permittivity of free space is denoted by ϵ. The externally applied force in the direction of motion is denoted

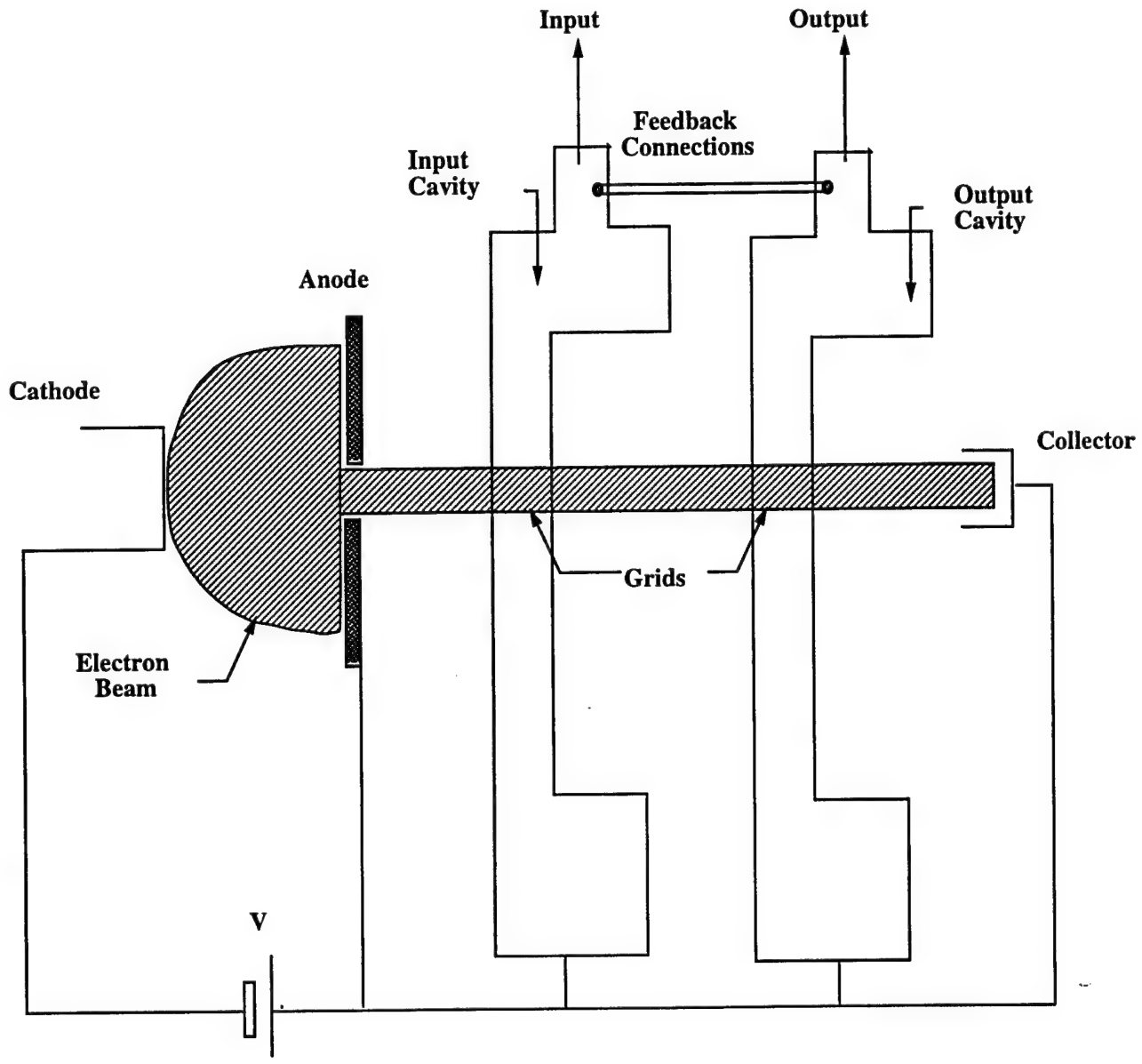

Figure 1. A conventional two–cavity klystron amplifier with positive feedback connections for use as an oscillator

by $F_{ext}(t) = eE(t)$, where $E(t)$ is the electric field in the direction of motion due to all sources (except the electron in question). We are using the International System of Units (mksA) throughout.

The first term on the right-hand side of (11) represents the relativistic generalization of Newton's second law of motion. The second term on the right-hand side of (11) is the self-force on the electron in question generated by the acceleration (and its time derivative).[1] This self-force term is usually neglected in particle-in-cell computer codes. Here, we want to determine if the self-force term is indeed negligibly small.

We can greatly simplify the estimation of the self-force by moving to an inertial frame of reference K' moving with the average speed u_0 of the electrons. In this K' frame of reference, the velocity of the electrons can be approximated by a sinusoidal function

$$u' = u'_1 \cos \omega' t' \tag{13}$$

where t' is the time measured in the K' frame, u' is the velocity of the electron in the K' frame (u'_1 is a constant and $u'_1 \ll c$), and ω' is the frequency of operation of the HPM device as measured in the K' reference frame. It is related to the frequency ω measured in the laboratory frame through the relativistic transformation

$$\omega' = \gamma_0 \omega \tag{14}$$

with

$$\gamma_0 = \frac{1}{\sqrt{1 - u_0^2/c^2}}. \tag{15}$$

Moreover, in the K' frame, the equation of motion (11) simplifies to [4, eq. (3.3)]

$$F'_{ext} = m\frac{du'}{dt'} - \frac{e^2}{6\pi\epsilon c^3}\frac{d^2u'}{dt'^2} \tag{16}$$

since $u'_1/c \ll 1$.

[1]The second term in (11) is not identical in form to that of the self-force term in [4, eq. (5.12a)] because the self-force term in equation (5.12a) of [4] reduces to the self-force term shown in (11) for rectilinear motion.

The equation of motion (16) can be written as

$$F'_{ext} = F'_N - F'_S \tag{17}$$

where

$$F'_N = m\frac{du'}{dt'} \tag{18}$$

is the usual Newtonian acceleration force of the electron and

$$F'_S = \frac{e^2}{6\pi\epsilon c^3}\frac{d^2u'}{dt'^2} \tag{19}$$

is the self-force on the electron. The self-force will be negligible compared to the Newtonian acceleration force if

$$\frac{< |F'_S| >}{< |F'_N| >} = \frac{e^2 < |d^2u'/dt'^2| >}{6\pi\epsilon c^3 m < |du'/dt'| >} \ll 1 \tag{20}$$

where the brackets $< >$ indicate the average per cycle. From (13) we find that (20) reduces to

$$\frac{e^2\omega'}{6\pi\epsilon c^3 m} \ll 1 \tag{21}$$

or with the help of (14)

$$\omega \ll \frac{6\pi\epsilon c^3 m}{e^2\gamma_0} \tag{22}$$

or

$$\omega \ll \frac{1.6 \times 10^{22}}{\gamma_0}. \tag{23}$$

In HPM devices, γ_0 is usually on the order of 10 or less. Even in the largest accelerators, γ_0 is seldom greater than a few thousand. Thus, one sees from (23) that the HPM device would have to operate at gamma-ray frequencies before the self-force became appreciable.

2.2 Neglect of self-force in PIC computer codes

In the previous section we showed that the self-force on individual electrons in HPM devices was negligible compared with the Newtonian acceleration force. However, in particle-in-cell

computer codes, many electrons are grouped together into one cell and each of these groups of electrons are treated as a single point particle with rest mass M and charge Q. Nonetheless, since M and Q represent the total mass and charge of a cell of N_e electrons, they are given by

$$M = N_e m\,, \quad Q = N_e e. \tag{24}$$

Moreover, for each electron in the cell we can repeat the analysis of the previous section to obtain a total Newtonian acceleration force on all the electrons in the cell equal to $N_e F'_N$ and a total self-force on all the electrons in the cell equal to $N_e F'_S$. Thus, the self-force on the "particle-in-cell" is negligible compared to the total Newtonian acceleration force if

$$\frac{< |N_e F'_S| >}{< |N_e F'_N| >} = \frac{< |F'_S| >}{< |F'_N| >} \ll 1 \tag{25}$$

or, from (20)-(23), if

$$\omega \ll \frac{6\pi\epsilon c^3 m}{e^2 \gamma_0} = \frac{1.6 \times 10^{22}}{\gamma_0}. \tag{26}$$

In other words, whether for a single electron or a group of electrons composing a particle-in-cell, the self-force is negligible for frequencies of operation less than gamma-ray frequencies.

One subtlety that should be mentioned concerns the mass M of the particle-in-cell composed of N_e electrons. We have assumed that this mass is given simply by $M = N_e m$, where m is the mass of each electron. One could point out that to this mass should be added a mass of formation needed to bring the N_e electrons together in one cell from an infinitely large separation distance. However, since the cell is assumed small enough that all the electrons in each cell move together in the HPM device with little mutual electromagnetic repulsion, the energy of formation needed to overcome this mutual repulsive force between the electrons in any one cell is also negligible. Thus, the mass of formation, equal to the energy of formation divided by c^2, is also negligible.

2.3 The Effect of the Self-Force on a Charge Moving in a Constant, Uniform Electric Field between Two Charged Parallel Plates

In this section we shall prove a rather remarkable result [5, Secs. 5-3, 6-11]: The self-force term in the equation of motion completely vanishes for a charge (e.g., an electron) moving in the direction of a constant, uniform electric field such as the electric field produced between two oppositely charged parallel plates. As a consequence of this result, the motion of the electron, beginning at rest on the negatively charged plate (cathode), can be described exactly by the relativistic version of Newton's second law of motion.

To prove the former result, write the Lorentz-Abraham-Dirac equation of motion (11) for an electron moving with velocity $u(t)$ in the direction of and applied constant, uniform electric field E_0, so that $F_{ext} = eE_0$ in (11):

$$eE_0 = m\frac{d}{dt}(\gamma u) - \frac{e^2}{6\pi\epsilon c^3}\gamma^4\left[\frac{d^2u}{dt^2} + \frac{3\gamma^2}{c^2}u\left(\frac{du}{dt}\right)^2\right]. \tag{27}$$

One can show [4, ch. 8] that the substitution

$$\gamma u = c\sinh(\mathcal{V}/c) \tag{28}$$

converts (27) to

$$eE_0 = m\frac{d\mathcal{V}}{d\tau} - \frac{e^2}{6\pi\epsilon c^3}\frac{d^2\mathcal{V}}{d\tau^2} \tag{29}$$

where $d\tau = dt/\gamma$ and

$$\gamma = (1 - u^2/c^2)^{-\frac{1}{2}} = (1 + \sinh^2(\mathcal{V}/c))^{\frac{1}{2}} = \cosh(\mathcal{V}/c). \tag{30}$$

The solution to (29), with E_0 independent of time and thus independent of τ, can be found by inspection to be

$$\frac{d\mathcal{V}}{d\tau} = \frac{eE_0}{m}. \tag{31}$$

Because $d\mathcal{V}/d\tau$ equals a constant, $d^2\mathcal{V}/d\tau^2 = 0$ and (29) is satisfied. But since $d^2\mathcal{V}/d\tau^2 = 0$, the second term on the right-hand side of (27) is zero and (27) can be written simply as

$$eE_0 = m\frac{d}{dt}(\gamma u). \tag{32}$$

That is, the motion of the electron moving in the direction of a constant, uniform electric field is determined completely by the relativistic second law of motion (32), because the self-force in this constant, uniform electric field is identically zero.

One can explain this strange and remarkable result by dividing the self-force term into two terms, an irreversible radiation reaction term and a reversible "Schott acceleration" term [4, ch. 7]

$$\gamma^2\left[\frac{d^2u}{dt^2} + \frac{3\gamma^2}{c^2}u\left(\frac{du}{dt}\right)^2\right] = -\frac{\gamma^6 u}{c^2}\left(\frac{du}{dt}\right)^2 + \frac{d}{dt}\left(\gamma^4\frac{du}{dt}\right). \tag{33}$$

The first term on the right-hand side of (33) is the irreversible radiation-reaction force cause by the momentum radiated by the electron being accelerated in the applied electric field. The second term is the reversible "Schott acceleration" force. It behaves as a reactive force that draws momentum from the reactive fields of the accelerating electron. For a charge moving in the direction of an applied constant, uniform electric field, these two terms cancel. That is, the momentum radiated by the accelerating electron produces a retardation force on the electron that is just cancelled by the rate of change of momentum that the electron draws from its reactive fields. Of course, when the electron collides with the positive plate (anode), or travels through a hole in the positive plate into the force-free region, the reversible Schott momentum and energy is taken from the electron, leaving only the momentum and energy imparted by the applied electric field less the radiated momentum and energy.

2.4 Solution to equation of motion for an electron traveling between two oppositely charged parallel plates

We have just shown that the motion of an electron traveling in the direction of the electric field between two oppositely charged parallel plates is described by the relativistic second law of motion (32). Let us solve this equation of motion for the velocity of the electron. Assume the electron starts at rest at the cathode, and that the parallel plates (anode and cathode) are oppositely charged to a voltage V_0. Let us find the final velocity u_f as the electron reaches the anode, which is separated from the cathode by a distance d.

Multiplying (32) by u, one finds that

$$mc^2\frac{d\gamma}{dt} = eE_0u = eE_0\frac{dx}{dt} \tag{34}$$

where x is the distance of travel between the plates. Integrate (34) from $x = 0$ (the cathode) to $x = d$ (the anode) to get

$$mc^2(\gamma_f - 1) = eE_0d = eV_0\ , \quad \gamma_f = (1 - u_f^2/c^2)^{-\frac{1}{2}} \tag{35}$$

or

$$\frac{1}{\sqrt{1 - u_f^2/c^2}} = \frac{eV_0}{mc^2} + 1. \tag{36}$$

Solving (36) for the final velocity u_f, we find

$$u_f = c\sqrt{1 - (eV_0/(mc^2) + 1)^{-2}} \tag{37}$$

or

$$u_f = c\sqrt{1 - (1.9569 \times 10^{-6}V_0 + 1)^{-2}}. \tag{38}$$

For example, if $V_0 = 350,000$ volts, the electron will be traveling at a speed of

$$u_f = .80484c \tag{39}$$

as it reaches the anode. As will be discussed below in Section 2.6, this result was confirmed with the Sandia National Laboratories, Albuquerque PIC code TWO-QUICK.

2.5 Alternate approaches to the PIC scheme

In an attempt to explore schemes that might be more effective for microwave source production involving ultra-relativistic sources, we began exploring alternate approaches to these PIC algorithms. In particular, we considered one approach which is a one-step scheme in 0 to the usual two-step field-solve / particle-push approach. The second scheme we considered is in principle a two-step scheme but one which could potentially be more accurate for relativistic particle pushing.

First we considered a continuous distribution of moving charges characterized by a charge density $\rho_q(\vec{r},t)$, a mass density $\rho_m(\vec{r},t)$, and a velocity $\vec{v}(\vec{r},t)$. We note first that the mass and charge densities are related by the expression

$$\rho_m(\vec{r},t) \;=\; \frac{m}{q}\,\rho_q(\vec{r},t)\,. \tag{40}$$

Also the current can be written in the form

$$\vec{J}(\vec{r},t) \;=\; \rho_q(\vec{r},t)\,\vec{v}(\vec{r},t) = \vec{v}(\vec{r},t)\,\nabla\cdot(\epsilon\vec{E}(\vec{r},t))\,. \tag{41}$$

Maxwell's equations can then be rewritten in a homogeneous medium in the form

$$\begin{aligned}\nabla\times\vec{E} &= -\frac{\partial}{\partial t}\vec{B}\\ \nabla\times\vec{B} &= \epsilon\mu\left(\frac{\partial}{\partial t}+\vec{v}\cdot\nabla\right)\vec{E}\,.\end{aligned} \tag{42}$$

The force equation takes the form

$$\vec{E}+\vec{v}\times\vec{B} \;=\; \frac{m}{q}\left(\frac{\partial}{\partial t}+\vec{v}\cdot\nabla\right)(\gamma\vec{v})\,. \tag{43}$$

Writing the magnetic induction field in the form

$$\vec{B} \;=\; -\int^t \nabla \times \vec{E}\, dt' \,. \tag{44}$$

one is led to the equations

$$\begin{aligned} -\nabla \times \nabla \times \int^t \vec{E}\, dt' \;&=\; \epsilon\mu \left(\frac{\partial}{\partial t} + \vec{v}\,\nabla\cdot\right) \vec{E} \\ \vec{E} - \vec{v} \times \nabla \times \int^t \vec{E}\, dt' \;&=\; \frac{m}{q} \left(\frac{\partial}{\partial t} + \vec{v}\cdot\nabla\right) (\gamma\vec{v}) \,. \end{aligned} \tag{45}$$

from which one can write the velocity as

$$\begin{aligned} \vec{v} \;&=\; -\frac{1}{\nabla\cdot\vec{E}} \left(\frac{1}{\epsilon\mu}\,\nabla \times \nabla \times \int^t \vec{E}\, dt' + \frac{\partial}{\partial t}\vec{E}\right) \\ &=\; \frac{1}{\nabla\cdot\vec{E}} \left(\frac{1}{\epsilon\mu}\nabla \times \vec{B} - \frac{\partial}{\partial t}\,\vec{E}\right) \,. \end{aligned} \tag{46}$$

It is immediately apparent that the expression for the velocity leads to a highly nonlinear system of equations. In particular, one obtains in terms of the electric field $\vec{E}$ alone:

$$\begin{aligned} \vec{E} + \frac{1}{\nabla\cdot\vec{E}} \left(\frac{1}{\epsilon\mu}\,\nabla \times \nabla \times \int^t \vec{E}\, dt' + \frac{\partial}{\partial t}\vec{E}\right) \;\times\; \nabla \times \int^t \vec{E}\, dt' \\ = \; \frac{m}{q} \left(\frac{\partial}{\partial t} + \vec{v}\cdot\nabla\right) (\gamma\vec{v}) \,. \end{aligned} \tag{47}$$

or, alternatively, in terms of $\vec{E}$ and $\vec{B}$:

$$\vec{E} + \frac{1}{\nabla\cdot\vec{E}} \left(\frac{1}{\epsilon\mu}\nabla \times \vec{B} - \frac{\partial}{\partial t}\,\vec{E}\right) \times \vec{B} \;=\; \frac{m}{q} \left(\frac{\partial}{\partial t} + \vec{v}\cdot\nabla\right) (\gamma\vec{v}) \,. \tag{48}$$

Because it has been embedded in (47) or (48), the Lorentz force equation need not be considered explicitly. Discretization of both systems was attempted without much success for practical implementation. Explicit and semi-implicit update equations can be derived from (47) or (48). System (47) has too many curl operations to maintain a nice local stencil; system (48) has a similar problem due to the cross products. Nonetheless, they provide an alternative approach to obtaining the desired field quantities without having the intermediate step of the particle-push.

An alternative two-step approach was also investigated. If we consider the 0 particle equations in the presence of an electromagnetic field:

$$\begin{aligned} \frac{d}{dt}x^\mu &= \frac{p^\mu}{\gamma m} \\ \frac{d}{dt}p^\mu &= \frac{q}{\gamma m} F^\mu_\nu \, p^\mu \end{aligned} \tag{49}$$

where F^μ_ν represents the anti-symmetric electromagnetic field tensor, their solution can be written in terms of an explicit integration as

$$\begin{bmatrix} x^\mu(t) \\ p^\mu(t) \end{bmatrix} = \begin{bmatrix} 1 & \int_0^t \frac{1}{\gamma m} \exp\left(\frac{q}{\gamma m} F^\mu_\nu s\right) \, ds \\ 0 & \exp\left(\frac{q}{\gamma m} F^\mu_\nu t\right) \end{bmatrix} \begin{bmatrix} x^\mu(0) \\ p^\mu(0) \end{bmatrix}. \tag{50}$$

This generates a solution in the eight dimensional phase space of the particles. The matrix operator can actually be reduced analytically using Lorentz group Lie algebra to achieve an explicit integrator. This would have the advantage of preserving the consistency between the momentum and energy conservation equations, i.e., the force equation and the equation for the 0 γ term. The usual leap-frog procedure discussed in Section 1 can lead to numerical

inaccuracies if these quantities become out-of-sync with each other. This explicit phase space integrator would circumvent these potential inaccuracies.

In principle, one could rewrite the entire Maxwell-Lorentz system into such an explicit matrix integration scheme. This approach would be a single-step approach and it would have many advantages since all the field and particle quantities would be integrated forward in time simultaneously. Unfortunately, this approach appears to have a high cost in terms of its memory requirements. For instance, even for the state space system, the update for $x^{\mu}(t)$ at each point in the grid would encompass a running sum of the field at every point in the grid. On the other hand, it may be possible to adapt this approach to include the effects of radiation damping by using the more general force equation given in [4]. However, as shown in 2.2, these self-forces can be neglected and the Newtonian force is sufficient for HPM purposes.

2.6 PIC Code Validation

The TWO-QUICK PIC code was acquired from Sandia National Laboratories - Albuquerque (SNLA). This simulation software also required installation of IDL; it acts as the graphical user interface (GUI) for the TWO-QUICK PIC code. The documentation associated with this code is minimal. The TWO-QUICK code developers were very generous with their thoughts and time on how to get started running the code. Nonetheless, the learning curve was steep even to try some simple examples.

Because of the costs associated with these PIC simulations, only a variety of simple test problems were run; the results agreed with basic physics principles and solutions. No 0 results for simple problems were found, especially for the parallel-plate case discussed in 2.4. In particular, the parallel-plate problem was run with a minimum of two particles (the

particle generation routines in TWO-QUICK would not permit a single particle test case) and with several thousand (to see if the particle statistics mattered). The energy and particle fluxes at the anode were measured to extract the information needed to calculate the velocity of the particles at the anode. For the two electron case the code predicted the final particle velocities at the cathode to be $v = 0.80402c$ rather than the analytical value of $v = 0.80484c$, a 0.1% error. With many particles, the result changed trivially. Thus, the TWO-QUICK code reproduced the analytical values to a very high degree of precision.

The parallel-plate case is actually a very difficult problem for most PIC codes since it is basically an electrostatic problem that mainly exercises the particle-push algorithm. There were several different ways to set up this problem and the information produced comes in several different forms. As with any PIC code, care needs to be exercised in running the code. Special considerations must be given to the spatial grid size, the corresponding time step sizes, the number of particles in the simulation, and the types of sources used to generate the particles. Moreover, since much of the post processing information is in the form of particle fluxes, energies, momentums, etc., for the discrete particles, care must be exercised in using the output quantities correctly to obtain the desired values. Nonetheless, experienced users with a well-validated PIC code can produced reliable values for the quantities of interest.

3 Conclusions

The effects of the self-force in PIC calculations were considered. It was explicitly demonstrated that the usual Maxwell-Lorentz equation system does not suffer from the lack of a self-force treatment in the particle-push stage of the PIC solution process. In particular, the self-force was estimated and found to be negligible in HPM applications for frequencies less than gamma-ray frequencies. We also used the SNLA PIC code TWO-QUICK to simulate

the final velocity of a single particle traveling between two oppositely charged parallel plates. The simulated final velocity agreed with the exact analytically derived final velocity to within 0.1%. Several alternative approaches to treating the Maxwell-Lorentz system numerically were also considered. It was found that the standard two-stage, particle-push and field-solve, scheme is one of the most efficient numerical approaches one can apply to modeling plasmas in high power microwave devices. The alternative single-stage approaches may, in principle, produce more accurate results, but they are not presently amenable to a practical numerical implementation.

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